Electron-phonon interaction in two dimensions: The case for strong coupling in high-T_c superconductors

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A particular model interaction between electrons and acoustic phonons is found to cause electrons to become weakly "self-trapped" for an arbitrary filling factor in $d=2$, but not in $d=1$ nor, for different reasons, in $d \geq 3$. To the extent that electron kinetic energy is reduced in $d=2$, the electronic *interactions* become proportionally more effective. Among phonon-mediated interactions we identify a static anisotropic interaction, compatible with observed ordering of oxygen vacancies along privileged axes in $YBa_2Cu_3O_{7-x}$, while other mechanisms encourage electron pairing and superconductivity.

Motivated by startling experimental developments, theorists have recently been rushing to propose any number of explanations for high-T_c superconductivity. The present paper originated in observations[1] that this phenomenon occurs principally in quasi-two-dimensional materials of low conductivity. The model electron-phonon interaction that I study here differs from many conventional pictures in that electrons are centered on bonds, halfway between metallic atoms—just where the oxygen atoms are—and not *on* the metallic atom sites. With this proviso, it leads to electron "quasi-self-trapping," but only in two dimensions. It follows that if the effective bandwidth is small, or zero, the electronic interactions are relatively that much stronger, and phenomena which depend on interactions are that much more effective.

Effective dimensionality is here determined, not by the electron motion, but by the long-wavelength phase space available to acoustic branch phonons. Even if a material is physically three dimensional, the acoustic branches associated with certain stretching modes (intraplanar elastic parameter K) can be effectively two dimensional if the interplanar coupling $K_z \ll K$, and this will suffice for our purposes. If the theory is correct, the role of Y or other rare-earth metals in the family of high-T_c superconductors such as $YBa_2Cu_3O_{7-x}$ may just be that of a buffer, isolating lattice vibrations in the separate atomic planes from one another.

When an electron is removed from halfway between two Cu atoms separated by a distance a_0, the *intermetallic* separation relaxes to a new equilibrium value, say a_1. (The position of the oxygen atom midway between the atoms is unaffected.) When the same electron is returned to a nearby link of length a_1, this latter relaxes to a_0 by an inverse process. In a *linear* chain molecule, the resulting phonon drag reduces the hopping matrix elements t to a lesser value t', thereby diminishing the bandwidth of the electrons or holes by a corresponding amount. Because of certain cancellations, there are no singularities whatever, and the renormalized t' can never be identically zero. In a square lattice in two dimensions, nearest-neighbor (NN) bonds are *perpendicular* to one another (see Fig. 1), thus their stretching modes are mutually orthogonal. If the cancellations operative in $d=1$ are absent, the infrared singularity in the cloud of acoustic modes surrounding the particle in $d=2$ causes the NN electron parameter t' to vanish regardless of how small the electron-phonon coupling constant might be. Thus, according to our model, the square (SQ) lattice with nearest-neighbor hopping is *inherently* in the strong-coupling regime.

Next-nearest neighbor (NNN) hopping between paral-

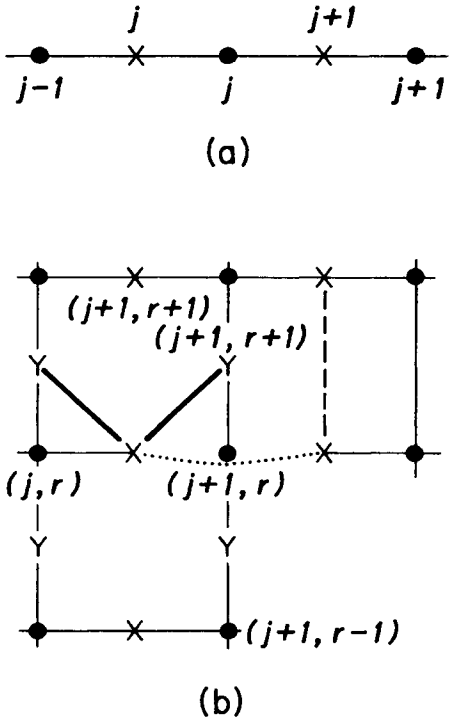

FIG. 1. Top: $d=1$ (linear chain) atoms are filled circles; electrons are crosses. Bottom: $d=2$ (SQ lattice). Metal atoms are vertices, electrons (as well as oxygen sites) indicated by x (on horizontal bonds) and y (vertical). (——) Nearest neighbor ($x \rightarrow y$) hop shown, (---) interchain next-nearest neighbor, and (....) intrachain next-nearest neighbor.

lel bonds restores nonzero but anisotropic value to the renormalized hopping parameter t'. Correlated electron-phonon ("polaron") hopping also tends to restore the particles' ability to move.

Even if the identical mechanism were operative for electrons on a $d=3,4,\ldots$ lattice, the phase space factor k^{d-1} at $k=0$ cures the mild singularity in $d>2$. Unless the coupling constant is unusually large, this creates a presumption of weak coupling for the electron-phonon interaction of our model in all $d\geq 3$.

The electron-phonon interaction has a secondary effect which appears only when the fields are decoupled. The decoupling causes a static electron-electron potential $V_K(\mathbf{R}-\mathbf{R}')$ to appear, one which is highly anisotropic and oscillatory, and independent of atomic masses M. This comes about independent of the electrons' motions, and applies equally to such other "particles" as holes and oxygen vacancies occupying the same Cu—Cu bonds. The oscillations and anisotropy of V_K could well cause the long-range uniaxial orderings observed for the fraction x of oxygen vacancies[2] in $YBa_2Cu_3O_{7-x}$. The exact character of V_K depends on d; it is reasonably long ranged in $d=2$, but increasingly shorter ranged for $d=3,4,\ldots$. Surprisingly, V_K is identically zero in $d=1$. While it is not clear that V_K can promote Cooper pairing and/or superconductivity[3] of electrons for sufficiently large spring constant K, it does provide a specific mechanism for the interaction of defects with one another and with electrons or holes. An exposition of the superconducting aspects will be given in a separate paper under preparation.[4] For simplicity, we start with $d=1$.

$d=1$. In a linear-chain molecule with electrons localized on links, only atomic motions parallel to the chain (say, the x-direction) are relevant and the phonon Hamiltonian takes the form

$$H_{\rm ph}=\tfrac{1}{2}M\sum_j p_{x,j}^2+(K/2)\sum_j (x_{j+1}-x_j-\gamma_j)^2 \ , \quad (1)$$

where x_j is the deviation from equilibrium ja_1, $p_{x,j}=(\hbar/i)\partial/\partial x_j$, and

$$\gamma_j=(a_0-a_1)\mathbf{n}(j) \ , \quad (2)$$

with $\mathbf{n}(j)\equiv n_+(j)+n_-(j)$, and $n_\sigma(j)=c_\sigma^*(j)c_\sigma(j)$, the electron occupation number for spin direction $\sigma=\pm$. Although (1) apparently contains within it a form of electron-phonon coupling, the latter can be *entirely* eliminated by a canonical transformation:

$$x_j\rightarrow e^{iS}x_j e^{-iS}=x_j+\sum_{m<j}\gamma_m \ ,$$
$$S=\sum_j\sum_{m<j}\gamma_m p_{x,j}/\hbar \ . \quad (3)$$

This transformation takes $H_{\rm ph}$ into $H_{\rm ph0}$, the pure phonon Hamiltonian obtained from (1) by setting all γ's $=0$, and is then readily diagonalized as $H_{\rm ph0}\rightarrow\sum\hbar\omega_k(\alpha_k^*\alpha_k+\frac{1}{2})$ with $\omega_k=2\omega_D|\sin(k/2)|$, $\omega_D=(K/M)^{1/2}$. Although in $d=1$ the potential energy in this model is perfectly independent of where the electrons (if any) are located, the interaction *does* reappear in the form of a modification to the electron-transfer H_1:

$$H_1\equiv -t\sum_{j,\sigma}[c_\sigma^*(j+1)c_\sigma(j)+\text{H.c.}] \ , \quad (4)$$

which under (3) transforms into

$$H_1\rightarrow -t\sum_{j,\sigma}[c_\sigma^*(j+1)c_\sigma(j)e^{i[\Omega(j+1)-\Omega(j)]}+\text{H.c.}] \ , \quad (5)$$

with

$$\Omega(j)=g_0\sum_{r>j}[(1/N)^{1/2}\sum_k e^{ik\cdot r}|2\sin(k/2)|^{1/2}\alpha_k/i+\text{H.c.}] . \quad (6)$$

The lumped coupling constant is $g_0\equiv(a_0-a_1)(M\omega_D/2\hbar)^{1/2}$. Note that while $\Omega(j+1)$ is singular (when the sum over sites r is evaluated, the coefficient of $\alpha_k\rightarrow k^{-1/2}$ in the long wavelength limit), the *difference* $\Omega(j+1)-\Omega(j)$, which is what appears in the exponent, is not.

It remains to introduce the two-body Coulomb forces, $H_c(n(j))$, for a complete statement of the problem of a model linear chain.[5] H_c commutes with, and hence is unaffected by, the transformation (3) which simplified $H_{\rm ph}$ while complicating H_1. For a zeroth-order estimate of the effective bandwidth t', one thermally averages (TA) over the phonon coordinates:

$$t'\equiv t<e^{i[\Omega(j+1)-\Omega(j)]}>_{\rm TA}$$
$$=t\exp-\left[(g_0^2/N)\sum_k|2\sin(k/2)|(n_k+\tfrac{1}{2})\right] \quad (7)$$
$$\equiv t\exp[-\Phi(T)]$$

in which

$$n_k+\tfrac{1}{2}=(e^{\beta\hbar\omega}k-1)^{-1}+\tfrac{1}{2}\rightarrow k_BT/\hbar\omega_k$$

in the high-T limit. The particular form of (7) is the direct consequence of the cancellations of terms in $\Omega(j+1)-\Omega(j)$. Such cancellation, which occurs for electrons hopping between spatially parallel bonds, is inoperative for NN hopping in $d\geq 2$ as we shall now determine.

$d\geq 2$. In analyzing the SQ lattice (Fig. 1), at first we include only vertical and horizontal modes. Coupling of neighboring planes in a fully three-dimensional (3D) matrix will be discussed next. Labeling horizontal coordinates by integers j and vertical coordinates by integers r, i.e., $\mathbf{R}=(j,r)$, we write the phonon Hamiltonian which generalizes (1), $H_{\rm ph}=H_{{\rm ph},x}+H_{{\rm ph},y}$:

$$H_{{\rm ph},x}=\tfrac{1}{2}M\sum_j(p_{x;j,r})^2+(K/2)\sum_{j,r}[(x_{j+1,r}-x_{j,r}-\gamma_{j+1,r})^2+(x_{j,r+1}-x_{j,r})^2] \ ,$$
$$H_{{\rm ph},y}=\tfrac{1}{2}M\sum_j(p_{y;j,r})^2+(K/2)\sum_{j,r}[(y_{j,r+1}-y_{j,r}-\eta_{j,r+1})^2+(y_{j+1,r}-y_{j,r})^2] \ , \quad (8)$$

in which for notational clarity, $\gamma(\mathbf{R})$, i.e., $(a_0-a_1)\mathbf{n}_x(\mathbf{R})$ associated with particles on horizontal bonds is relabeled $\eta(\mathbf{R})$, $(a_0-a_1)\mathbf{n}_y(\mathbf{R})$, when it is associated with a vertical bond. The electron hopping operators take a particle from a γ site to a NN η site, or vice versa. Thus the electrons live effectively on a SQ bipartite lattice, oriented along 45° and 135° axes with lattice constant $a/\sqrt{2}$. After examining this, the distinctive changes effected by NNN hopping and interplanar interactions will be considered. There are significant changes from $d=1$.

(i) The canonical transformation S to decouple the γ's and η's from the lattice normal modes exists, but is less intuitive than (3).

(ii) For $d \geq 2$, the γ's and η's *cannot* be entirely eliminated.

After a bit of algebra[4] one is left with free phonons H_{ph0} [i.e., Eq. (8) with γ's and η's set $=0$],

$$\omega_k = 2\omega_D\sqrt{[\sin^2(k_x/2)+\sin^2(k_y/2)]} \ ,$$

plus a new contribution to the static electron-electron interactions denoted H_K:

$$H_K = \frac{1}{2}\sum_{\mathbf{R}}\sum_{\mathbf{R}'}[V_{1K}(\mathbf{R}-\mathbf{R}')\mathbf{n}_x(\mathbf{R})\mathbf{n}_x(\mathbf{R}')+V_{2K}(\mathbf{R}-\mathbf{R}')\mathbf{n}_y(\mathbf{R})\mathbf{n}_y(\mathbf{R}')] \ . \tag{9}$$

Actual calculation shows V_{1K} and V_{2K} to be anisotropic:

$$V_{1K}(\delta\mathbf{R}) = -(K)[(a_0-a_1)^2/N]\sum_k e^{i\mathbf{k}\cdot\delta\mathbf{R}}\sin^2(k_y/2)/[\sin^2(k_x/2)+\sin^2(k_y/2)]+\tfrac{1}{2}K(a_0-a_1)^2\delta(\delta\mathbf{R}) \ , \tag{10a}$$

with $\delta(\delta\mathbf{R})=1$ when $\delta\mathbf{R}=0$, and zero otherwise.

V_{2K} is a similar function rotated 90°:

$$V_{2K}(\delta\mathbf{R}) = -(K)[(a_0-a_1)^2/N]\sum_k e^{i\mathbf{k}\cdot\delta\mathbf{R}}\sin^2(k_x/2)/[\sin^2(k_x/2)+\sin^2(k_y/2)]+\tfrac{1}{2}K(a_0-a_1)^2\delta(\delta\mathbf{R}) \ . \tag{10b}$$

These potentials oscillate with the magnitude and orientation of $\delta\mathbf{R}$, starting from $V_{1K}(\mathbf{0})=V_{2K}(\mathbf{0})=0$. At any $\delta\mathbf{R}\neq\mathbf{0}$, we see $V_{1K}+V_{2K}=0$, thus where the one is attractive to the other is repulsive, while along the $(\pm1,\pm1)$ axes both vanish by symmetry.

Treating the oxygen vacancy in the same manner as the electrons (according to Fig. 1 the electrons are midway between Cu atoms, precisely where diagrams in various references[1,2] show the oxygen atoms to normally reside) with a slightly different definition of γ or η, leads to identical results, i.e., to an anisotropic vacancy–vacancy-interaction of the same form as (10) and may serve to explain the preferential uniaxial orderings of the vacancies. Lack of an observed oxygen isotope effect[6] is explained in the present model by the fact that the electronic motion does not correlate with the oxygen normal modes, which are orthogonal to the Cu—Cu bond stretching modes. On the other hand, interactions of electrons and oxygen vacancies via $V_K(\delta\mathbf{R})$ may be related to the enhancement or supppression of superconductivity.[7]

All V_K interactions obey the following rule: Horizontal defects interact only with other horizontals, verticals with verticals.

But this is not the end of the story; H_c and H_K are supplemented by *velocity-dependent* phonon exchange contributions H_1'' and H_2'' from the one-loop correction to H_1. H_1'' represents phonon-assisted hopping, and restores some width to the one-electron bands even in $d=2$. H_2'' may be the mechanism for Cooper pairing.[8]

The NN electron tight-binding Hamiltonian is given as

$$H_1 = -t_{xy}\sum_{\sigma}\sum_{(\mathbf{R},\mathbf{R}')}[c^*_{x\sigma}(\mathbf{R})c_{y\sigma}(\mathbf{R}')+\text{H.c.}] \ , \tag{11}$$

with $\mathbf{R}$ any site on the x sublattice and $\mathbf{R}'$ one of its NN on the y sublattice, distinguishing the fermion operators on the two sublattices as $c_{x\sigma}$ and $c_{y\sigma}$. Subsequent to the decoupling transformation, (11) becomes

$$H_1 = -t_{xy}\sum_{\sigma}\sum_{(\mathbf{R},\mathbf{R}')}[c^*_{x\sigma}(\mathbf{R})c_{y\sigma}(\mathbf{R}')e^{i[\Omega_K(\mathbf{R})-\Omega_y(\mathbf{R}')]}+\text{H.c.}] \ , \tag{12}$$

where

$$\Omega_K(\mathbf{R}) = g_0/(2N)^{1/2}\sum_k\{e^{i\mathbf{k}\cdot[\mathbf{R}-1/2,0)]}|\sin(k_x/2)|[\sin^2(k_x/2)+\sin^2(k_y/2)]^{-3/4}\alpha_{x,\mathbf{k}}/i+\text{H.c.}\} \tag{13a}$$

and

$$\Omega_y(\mathbf{R}') = g_0/(2N)^{1/2}\sum_k\{e^{i\mathbf{k}\cdot[\mathbf{R}'-(1/2,0)]}|\sin(k_y/2)|[\sin^2(k_x/2)+\sin^2(k_y/2)]^{-3/4}\alpha_{y,\mathbf{k}}/i+\text{H.c.}\} \ . \tag{13b}$$

It follows that the thermal average bandwidth in (12) is narrowed as

$$t'_{xy} = t_{xy}\exp(-g_0^2)(1/N)\sum_k[\sin^2(k_x/2)+\sin^2(k_y/2)]^{-1/2}(n_{\mathbf{k}}+\tfrac{1}{2}) \ . \tag{14}$$

The exponent diverges logarithmically at any $T > 0$, thus as a crude first approximation, $t'_{xy} = 0$. However, two factors can restore a modicum of electronic motility.

(i) There is phonon coupling into the third dimension, normal to the plane; because of the reduction in phase space, integrals such as in the exponent of (14) are greatly reduced. For $K_z \ll K$, one obtains

$$t'_{xy} \approx c t_{xy} (K_z/K)^{T/T_0} , \tag{15}$$

with T_0 and $c < 1$ lumped constants. Weak-coupling $K_z \ll K$ preserves the pseudo-2D character of the problem.

(ii) NNN hopping. If t_{xx} and t_{yy} are not initially zero, they will tend to be reduced by a small factor only, due to $d=1$ type cancellation [e.g., between $\Omega_x(\mathbf{R})$ and $\Omega_y(\mathbf{R}')$] for motion wholly within one sublattice. Although NNN motion is entirely within a given sublattice, evaluation of the exponents reveals it to be anisotropic. Detailed calculations to help understand diffusion kinetics of oxygen atoms in YBaCuO are under way.

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